Available online at www.sciencedirect.com
SCIENCE DIRECT®
Journal of Magnetism and Magnetic Materials 272–276 (2004) 941–942
Journal of magnetism and magnetic materials
www.elsevier.com/locate/jmmm

Local lattice symmetry of spin-glass and antiferromagnetic URh_2Ge_2

C.H. Booth[a,*], S.-W. Han[a], S. Süllow[b], J.A. Mydosh[c,d]

[a] *Chemical Sciences Division, Lawrence Berkeley National Laboratory, 1 Cyclotron Rd. MS 70A-1150, Berkeley, CA 94720, USA*
[b] *Institut fur Metallphysik und Nukleare Festkoerperphysik, TU Braunschweig, Braunschweig 38106, Germany*
[c] *Kamerlingh Onnes Laboratory, Leiden University, 2300 RA Leiden, The Netherlands*
[d] *Max Planck Institute for Chemical Physics of Solids, Dresden 01187, Germany*

Abstract

Polarized X-ray absorption fine-structure (XAFS) data are reported for Rh and Ge K edges on antiferromagnetic and spin-glass samples of URh_2Ge_2. Proposed crystal structures have two possible kinds of layers for the Rh and Ge atoms. The XAFS data indicate that each species forms both kinds of layers and therefore the dominant phase has a crystal structure like that of $CaBe_2Ge_2$.

PACS: 75.50.Lk; 75.30.Mb; 61.10.Ht; 71.27.+a

Keywords: URh_2Ge_2; Spin glasses; Heavy fermions; Disordered materials; XAFS

The physical properties of URh_2Ge_2 are interesting both from the point of view of a uranium-containing, heavy-fermion spin glass, and because this material has many properties in common with disordered non-Fermi liquids (NFL) [1], potentially indicating that the root of this behavior is similar to that of some NFL's. URh_2Ge_2 forms most easily into a spin glass (SG) ($T_F = 9$ K), but simple annealing can transform it into an antiferromagnet (AF) ($T_N = 13.4$ K) [1], providing evidence that lattice disorder generates the magnetic disorder necessary for the SG phase. In order to make real comparisons to other spin glasses and NFL's, the microscopic details of this system's unexpected lattice disorder need to be understood. In particular, even the average crystal symmetry is only tentatively identified as P4/nmm [2] ($CaBe_2Ge_2$-like), with I4/mmm ($ThCr_2Si_2$-like) among the other candidate structures. Below, we refer to these as the AS (asymmetrically stacked) and the SS (symmetrically stacked) models.

The X-ray absorption fine-structure (XAFS) technique can help clarify the situation. The Fourier transform (FT) of the normalized fine structure (χ) above an absorption edge is closely related to the radial bond length distribution around the absorbing atom. Moreover, since the final state of the photoelectron for a K edge has p symmetry, the XAFS have a directional dependence with respect to the incident photon polarization, $\hat{\boldsymbol{\epsilon}}$. Specifically, the XAFS amplitude is proportional to $(\hat{\boldsymbol{\epsilon}} \cdot \boldsymbol{r}_i)^2$, where $\boldsymbol{r}_i$ points along the direction to a neighboring atom. Therefore, by rotating the crystal defined in Fig. 1a with respect to $\hat{\boldsymbol{\epsilon}}$, one can enhance or remove signal corresponding to the near-neighbor pairs within the r-type layers. In this way, we can determine whether the Rh atoms sit only in r-type layers as in the SS model, or whether they also occupy s-type layers, as in the AS model.

Data were collected in fluorescence mode on single crystals of SG and AF samples at 30 K from the Rh and Ge K edges. The samples were rotated within 10° of $\hat{\boldsymbol{\epsilon}}//\boldsymbol{c}$ and again within 10° of $\hat{\boldsymbol{\epsilon}}//\boldsymbol{a}$. Fig. 1b shows simulations of Rh K-edge XAFS data for the two proposed models, calculated using the FEFF8 program

*Corresponding author. Tel.: +1-510-486-6079; fax: +1-510-486-5596.
E-mail address: chbooth@lbl.gov (C.H. Booth).

0304-8853/$ - see front matter © 2003 Elsevier B.V. All rights reserved.
doi:10.1016/j.jmmm.2003.12.011

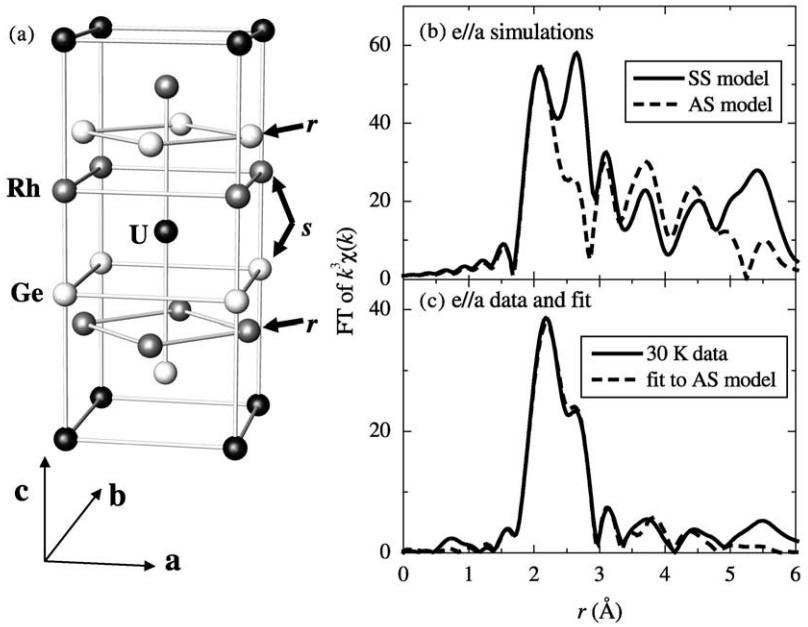

Fig. 1. (a) The proposed AS model for URh_2Ge_2. The SS-model structure is similar, with Ge occupying only s-type layers and Rh occupying only r-type layers. (b) Simulations of the Rh K-edge data with $\hat{\boldsymbol{\epsilon}}//\boldsymbol{a}$ assuming the two proposed lattice models. (c) Data on the antiferromagnetic sample with a fit to the AS model.

[4] with $\hat{\boldsymbol{\epsilon}}//\boldsymbol{a}$ (lattice vibrations only roughly included, lattice constants from Ref. [3]). The main peak at $\sim$2.2 Å in the transform is due to the Rh–Ge near neighbors between s- and r-type layers, corresponding to a pair distance of about 2.5 Å. The next peak at $\sim$2.6 Å is due to the Rh–Rh pairs within r-type layers with a pair distance of about 2.9 Å. This latter peak is not present with $\hat{\boldsymbol{\epsilon}}//\boldsymbol{c}$ for either the simulated or the measured data (not shown). In the SS simulation, all the Rh is in r-type layers, and the Rh–Rh (2.9 Å) scattering is maximized. In the AS simulation, this amplitude is reduced by half, since half the Rh atoms are in s-type layers. The measured data from the AF single crystal (Data was fit and reduced using standard methods outlined by Li et al. [5]; A self-absorption correction is also applied, as described by Booth and Bridges [5].) shown in Fig. 1c clearly has amplitude in this region of the transform that is more consistent with the AS simulation, and fits assuming the AS model are excellent. Moreover, the data from both orientations and from the Ge K-edge support the AS model over the SS model. A third possibility that allows for both Rh and Ge atoms in a single layer is also ruled out as the dominant phase, since the first large peak from the Rh (Ge) edge data is found to be predominantly Ge (Rh). This random-occupancy phase may partially account for any impurity phases, however. The data and results on the SG sample are very similar.

In conclusion, the XAFS data on both antiferromagnetic and SG samples are consistent with the dominant crystal phase of URh_2Ge_2 having Rh and Ge alternate between s- and r-type layers. Although XAFS is not sensitive to long-range structure, this stacking is like that of $CaBe_2Ge_2$. This lattice is unusual for the f-electron intermetallic 122's, which are usually like that of $ThCr_2Si_2$. Disorder relative to this phase as well as differences between the antiferromagnetic and SG samples will be the topic of a future paper.

This work is supported in part by the U.S. Department of Energy (DOE) under Contract No. DE-AC03-76SF00098. Data were collected at the Stanford Synchrotron Radiation Laboratory, a national user facility operated by Stanford University for the DOE, Office of Basic Energy Sciences.

References

[1] S. Süllow, et al., Phys. Rev. B 61 (2000) 8878.
[2] S. Süllow, et al., J. Magn. Magn. Mater. 226–230 (2001) 35.
[3] S. Süllow, Ph.D. Thesis, Leiden University, 1996.
[4] A.L. Ankudinov, et al., Phys. Rev. B 58 (1998) 7565.
[5] G.G. Li, F. Bridges, C.H. Booth, Phys. Rev. B 52 (1995) 6332;
C.H. Booth, F. Bridges, Phys. Scr., in press.